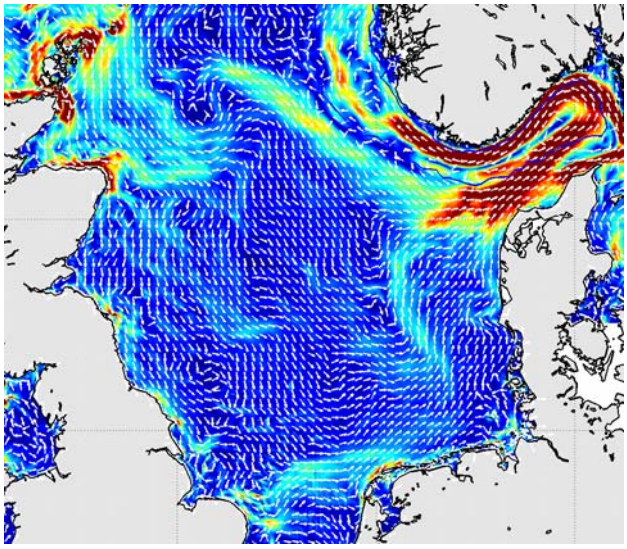
POLCOMS User Guide

V6.4

Jason Holt, March 2008



1. Introduction

Background

The origins of the Proudman Oceanographic Laboratory Coastal Ocean Modelling System (POLCOMS) lie with studies of frontal dynamics in the North sea for the UK NERC's North Sea Project. Since then it has been extensively developed both as a hydrodynamic and a multi-disciplinary model, including use of its sediment transport module, coupling to the European Regional Seas Ecosystem model and the Los Alamos Sea Ice model. Coupling to the GOTM model lends it a range of improved turbulence models. It has been used extensively in POL and PML's core research programme, and in on-going research contracts with the UK Met. Office and a wide range of NERC and EU funded research project and programmes, notably MERSEA, CASIX, MARPROD, LOIS, RAPID, ODON. It currently provides the 'work-horse' shelf sea model for the UK marine research centre programme: Oceans 2025, and the National Centre for Ocean Forecasting.

The scope of POLCOMS

POLCOMS is a three-dimensional baroclinic B-grid model designed for the study of shelf sea processes and ocean-shelf interaction. Recent work has taken it into estuarine environments. The model solves the momentum and scalar transport equations for oceanographic applications with realistic topography, bathymetry and forcing. The underlying hydrodynamics in POLCOMS are the shallow water equations with the hydrostatic and Boussinesq approximations. This limits models applicability to flows where the vertical acceleration is small and in practice this imposes a minimum horizontal resolution; simulation can be made at resolutions finer than this but at no benefit to the solution. As a rough guide this can be taken as half the maximum water depth.

Using this guide

This guide is aimed at providing a new user with a basic introduction to POLCOMS and to act as a reference for setting up new model domains. It lacks much of the details of the solution techniques, the most up-to-date reference for this is Holt and James [2001]; a full technical manual is in preparation.

POLCOMS is a complex model system and a large code (currently standing at around 95,000 lines of code) particularly resulting from the range of options and the parallel message passing code. To use it effectively requires an understanding of the model equations and boundary conditions, and how these are represented numerically and coded. While this document describes many of the options available nothing beats looking in the code to see what they do.

Throughout this guide the following typographic conventions are used:

- Variables in equations in italics e.g. *T*
- Variables names and code in bold e.g. **tmp**
- cpp compiler directives in bold capital e.g. **NOSCOORD**
- Subroutine/module names in bold italics e.g. ***b3drun***
- Filenames in bold Arial e.g. **b3drun.F**

The code

POLCOMS is available under license to collaborators of the Proudman Oceanographic Laboratory.

The model release 'un-tars' into the following directory structure:

pol3db

v6.3	The source code
PMLersemv2.0	
CICE	Additional model codes (available from the originators)
WAM	
setups	Application specific subdirectories
plume	
MRCS	
IRS	

The source code consists of:

- *.F - FORTRAN 90 (fixed format) source with cpp directives: the main body of code
- *.c - C source files (used for command line arguments and GUI)
- *.h - include files
- makefile - for compilation control
- objects_* - lists of source object files for POLCOMS and subsidiary models
- machine_list - machine_dependent options
- dependencies_pol3db - code inter-dependencies

Generally one set of source code is used for all applications, but there is the option of including application-specific code e.g. for different forms of data output.
The GOTM model should be installed as per instructions on www.gotm.net and is then used as a library.

2. Defining the problem

Unlike a global model, a regional ocean model is defined for a limited area and as such can take on a wide range of configurations and domains, each approaching the solution of the equations in a different fashion and being subject to different forcing. This requirement for flexibility is controlled in three ways in POLCOMS:

- cpp compiler directives are used to select portions of the code or exclude others (e.g. **-DNOSCOORD** selects σ-coordinates instead of s-coordinates). Many of these in fact set logical variables in **parm_defaults.F.** Compiler directives are most conveniently set in a compilation script specific for the application (e.g. **make_polcoms**).
- All logical variables defined in the main module (**b3d.F**) can be set in a name list file **logicalvariables.inp**. This overrides the logical variables set by compiler directives
- A number of run-time command-line arguments are available, to set properties such as length of model run, check-pointing, type of domain decomposition.

Current compiler directives are described in appendix A and options required for several example applications are listed described in appendix D

Control files

POLCOMS used a number of control files to set basic model parameters and define input/output files. These can be used in combination with the model described above to define the model application.

- **parameters.dat** defines the grid size, resolution and a number of model parameters. For the current format see the example in appendix C.
- **scoord_params.dat** defines parameters for the s-coordinate transform (if used).

An example is:

```
150.0d0          hc    )
  1.0d0          cc    ) S coordinate parameters
  5.0d0       theta    )
 0.25d0          bb    )
```

for an explanation of these see Holt and James [2001]

- **logicalvariables.inp**. A nameslist file setting the logical variables in **b3d.F**, see appendix A.
- **filenames.dat** sets the names of input and output files. The format is:

```
INPUT
<input files directory>                    Path to directory of input files
<numnames >                                Number of input files
<input file, 1>
.
.
<logical unit> <type> <filename>                  logical unit for filename
.
.
<input file, numnames>
OUTPUT
```

<numnames >	Number of output file names
<Idname >	Run identifier
<output file, 1>	
.	
.	
<logical unit> <type> <filename>	logical unit for **filename**
.	
.	
<output file, numnames>	

Data Types are

1. formatted
2. unformatted
3. unformatted, without input directory path

When the model is run it opens all input files in the given path with the given name at the given unit, and all output files with the suffix "Idname" to identify the run output. Output files are (by default) written to the directory the model is run in.

Note: the logical units read in here are only used for the purpose of opening the files; they must match those used in the code. These are usually set in **data_out.F** for output, see appendix E for input data units.

3. Defining a POLCOMS grid

As a finite difference model, the spatial discretization on which the equations are solved is especially important. In POLCOMS this is a B-grid on either spherical polar coordinates or Cartesian coordinates in the horizontal and terrain following coordinates in the vertical.

Horizontal discretization

In the horizontal POLCOMS uses a B-grid discretisation, so both components of velocity (u,v) are defined at u-points, half a grid box to the southwest of points where elevations, ζ and other scalar variables are defined: b-points (see Figure 1). The domain size is **icg=1..l, jcg=1..m**, with (1,1) being the southwest corner. All horizontal arrays have a halo of at least 1 point (i.e array size is at least **(0..l+1,0..m+1)**) to facilitate message passing and open boundary data. Figure 1 shows the arrangement of grid points. The grid resolution (**rdal,rdbe**) is set in **parameters.dat** either as an inverse angular resolution (in degrees) or in metres for Cartesian coordinates (with directive **FLAT**). The coordinates (lat/lon or Cartesian) of the southwest (bottom-left) elevation points (**alon0, alat0** at **icg=1,jcg=1**) are also set in **parameters.dat.**

IMPORTANT Because the model is coded for multiprocessor systems almost all the horizontal indices in the model code (apart from i/o) refer to the **LOCAL** arrays (i.e.

those on a particular processor) and range from **i=1,iesub** and **j=1,jesub**. The relation between **LOCAL** (i,j) and **GLOBAL** (icg,jcg) indices is:

icg=i+ielb-1

jcg=j+jelb-1

The model is designed to be highly flexible in its definition of coastal and open boundaries. Hence there are 7 masks used to define these:

ipexu =1 at u-point where calculations are conducted
ipexb =1 at b-point where calculations are conducted
ipexub =1 at a sea u-point (including coastal points)
ipexbb =1 at a sea b-point
iucoast =1 where u-point is coastal and velocities are evaluated by the lateral boundary condition (case-II boundaries only, see below)
incb =1 at an open boundary points (always on b-points).
incu =1 at sea u-points next to open boundaries

The distinction between **ipexb** and **ipexbb** arises because there can be points across boundaries that are sea points, but where model calculations are not conducted. Other more specialized masks (e.g. in the advection routines) are described in the subroutine documentation.

The bathymetry (**hs**) is read in at the b-points as an ASCII file by the subroutine ***hset***:

```
real*8 depth(l,m)
If (leader) then
read(13,*) ((depth(i,j),i=1,l),j=1,m)
endif
call dist  (leadid,depth,hs,1)
```

If the **flipbathy** logical variable is set then the array is read from north to south rather than south to north (the defualt).

There are two configurations available as to where the sea-land boundary lies on this grid.

case-I boundaries

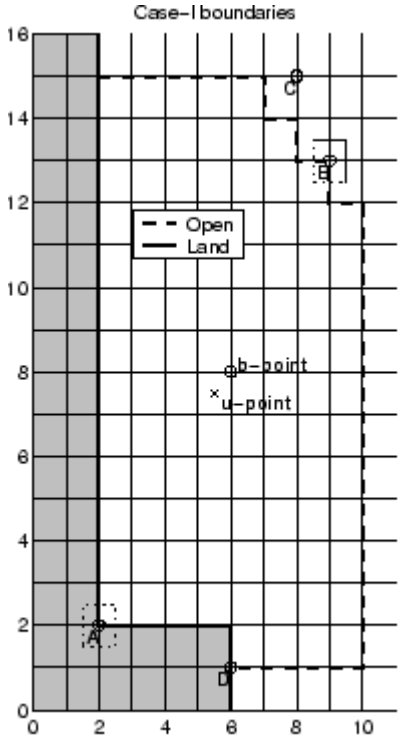
In this case land boundaries lie along b-points (Figure 1) and the primary definition of the land-sea grid is by the u-points (**ipexu**) which are either wholly land or sea. In the latter case each u-point is surrounded by four sea b-points, some of which may be fractional. This configuration implies a free-slip horizontal boundary condition, which is appropriate to all but fine resolution simulations. Most calculations occur at the coastal b-points (**ipexb(i,j)=1 h**ere), but the point is surrounded by a fractional grid box (**ar(i,j) = 0.5 or 0.25**). The grid is defined in ***boset*** by reading in **ipexu** (from an ASCII file in a similar

fashion to **hs**), then by setting **ipexb = 1** at all b-points surrounding a u-point where **ipexu = 1**. There is a test that the depth **hs** is non-zero at points with non-zero **ipexb**.

This configuration allows small islands and peninsulas to be included and gives a subgrid scale representation of the coastline, but wetting and drying is not available because of issues of volume conservation that would arise with fractional grid boxes. Model grid setups should use a procedure such as:

1. Define mask at u-points (**ipexu**) using the coastline (e.g. use GMT's command grdlandmask)
2. Calculate mask at b-points (**ipexb**)
3. Find bathymetry at sea b-points

Matlab (or similar) is useful for this and sometimes iteration from 3 to 1 is needed if the available bathymetry is not completely consistent with the available coastline.



A: i=2,j=2
ipexb(i,j)=1, ipexu(i,j)=0
ipexbb(i,j)=1, ipexub(i,j)=0
indb(i,j)=0, incu(i,j)=0
ar(i,j)=0.25

B: i=9,j=13
ipexb(i,j)=1, ipexu(i,j)=1
ipexbb(i,j)=1, ipexub(i,j)=1
indb(i,j)=1, incu(i,j)=1
ar(i,j)=1
ifaceob(2,i,j)=1, ifaceob(4,i,j)=1

C: i=9,j=14
ipexb(i,j)=0, ipexu(i,j)=0
ipexbb(i,j)=1, ipexub(i,j)=1
indb(i,j)=0, incu(i,j)=0
ar(i,j)=1

D: i=8,j=1
ipexb(i,j)=1, ipexu(i,j)=0
ipexbb(i,j)=1, ipexub(i,j)=0
indb(i,j)=1, incu(i,j)=0
ar(i,j)=0.5
ifaceob(1,i,j)=1

Figure 1 Case-I boundaries: coastal and open boundary lies along b-points.

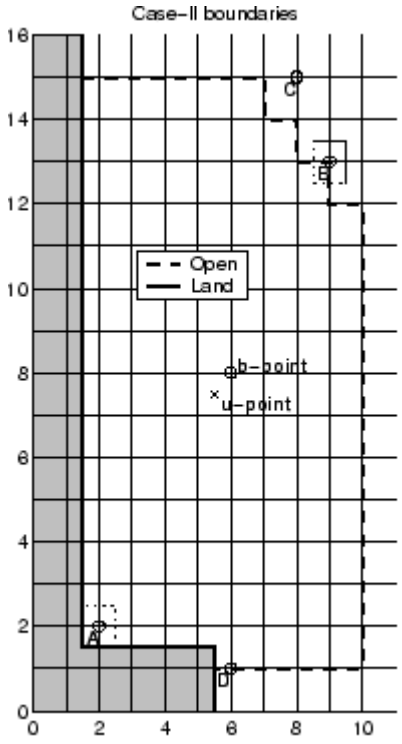
A simpler definition of case-I boundaries is available if sub-grid scale coastline representation is not required. In this case (compiler directive **SIMPLECASEI**) only a bathymetry file is used (no mask file), which defines **ipexb; ipexu=1** is then defined when all four surrounding b-points have **ipexb=1**.

An alternative method of defining the grid/water depth is provided by the logical options **analytic-depth.** In this case FORTRAN files called **set_bathymetry.F** and

set_maks.F are 'included'. These adjust set the global arrays **depth** and **mask** respectively.

case-II boundaries

In this case land boundaries lie along u-points (Figure 2). Calculations do not occur at the boundary points, but rather a lateral boundary condition is used, either non-slip (default) or slip (zero horizontal gradients are imposed with compiler directive **UBC**). In this configuration the bathymetry is used to set **ipexb** (where **hs** > **land**), then **ipexu = 1** if no surrounding **ipexb = 0**. At coastal grid points **ipexub = 1** and **ipexu = 0**. Hence all masks are derived from the bathymetry (no extra mask file is required) and this significantly simplifies model setup. This case allows wetting and drying to be implemented but the need for a horizontal velocity boundary condition is not desirable for coarser resolution simulations.



A: i=2,j=2
ipexb(i,j)=1, ipexu(i,j)=0
ipexbb(i,j)=1, ipexub(i,j)=1
incb(i,j)=0, incu(i,j)=0
ar(i,j)=1, iucoast(i,j)=1

B: i=9,j=13
ipexb(i,j)=1, ipexu(i,j)=1
ipexbb(i,j)=1, ipexub(i,j)=1
incb(i,j)=1, incu(i,j)=1
ar(i,j)=1
ifaceob(2,i,j)=1, ifaceob(4,i,j)=1

C: i=9,j=14
ipexb(i,j)=0, ipexu(i,j)=0
ipexbb(i,j)=1, ipexub(i,j)=1
incb(i,j)=0, incu(i,j)=0
ar(i,j)=1

D: i=8,j=1
ipexb(i,j)=1, ipexu(i,j)=0
ipexbb(i,j)=1, ipexub(i,j)=0
incb(i,j)=1, incu(i,j)=0
ar(i,j)=1, iucoast(i,j)=1
ifaceob(1,i,j)=1

Figure 2 Case-II coastal boundaries: coastal points lie alone u-points and open boundary lies along b-points.

Open boundaries

Open boundaries always lie along b-points (with either case-I or case-II coastal boundaries), but any point within the domain can be an open boundary point. Open boundary b-points are indicated by the **incb** array and the array **ifaceob** stores which faces of an open boundary point are open (i.e. receive fluxes from outside the model domain). By default any point with **ipexb(i,j)=1 at icg=1, icg=l, jcg=1, jcg=m** is an open boundary point (this means with case-I boundaries there can not be a coast-line along these rows/columns, since **ipexb = 1** on the coast - the model domain must be extended to

accommodate this). In addition to these default points a list of points can be read in of which faces around any model points are open boundaries (if the directive **READOPENBCPOINTS** is set). This reads the ASCII file **openbcpoints.dat**, which has the format

npts
icg jcg iface(1)
.
.
.
icg jcg iface(npts)

where **npts** is the number of additional open faces and the columns list the position of these (**icg,jcg**), and which face is open:

iface = 1 south
iface = 2 north
iface = 3 west
iface = 4 east

This allows any shaped open boundary to be defined.

Vertical discretization

The model uses a staggered vertical grid (Figure 3) with state variables defined 1/2 a grid box above and below the sea surface and bed, and flux variables defined at the surface and sea bed. Vertical indexing for the state variables is **k=2…n-1** (**k=1** and **k=n** are used for boundary conditions), and for flux variables is **k=1..n-1,** from the sea bed to the surface.

The model vertical coordinate is written in σ-coordinates, but there are two choices of how the model levels are discretized in σ-space:

- S-coordinates The level spacing in σ-space can vary in the horizontal; vertical coordinate variables **ds, dsu, sig, sigo** have 3 indices, and separate variables are defined at u-points: **dsv, dsu, sig, sigo**.
- σ-coordinates The level spacing in σ-space is fixed in the horizontal.

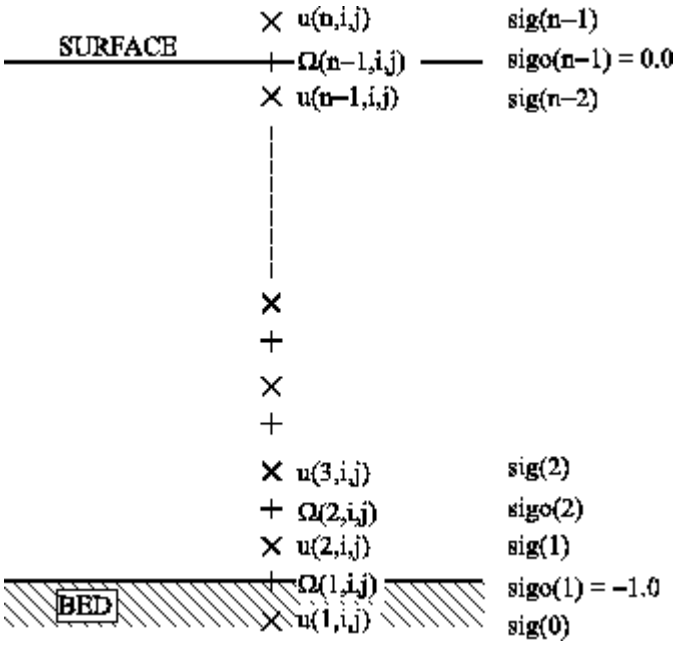


Figure 3 Vertical discretization

Hence in s-coordinates, state variables on b-points (e.g. **tmp(k,i,j)**) are defined at **sig(k-1,i,j),** are separated by **dsu(k-1,i,j)** and are associated with a depth, **ds(k-1,i,j).** Note: the difference in indexing of -1 from state variables is a historical anomaly which will be corrected in a future version.

Initial conditions

POLCOMS simulations generally start from rest with a level sea surface ($u=v=\zeta=0$), currently there are no provisions to initialise the model currents elevations except with a re-start files. The scalar fields on the other hand, are either initialised to a constant value (the default), read in from a file or specified from an 'included' piece of FORTRAN code.

With no options the initial T and S are set to the values given in **parameters.dat**. With directive **READ_INITIAL_TS** set they are read from unit 16 according to the format specified by **ts_form** in **parameters.dat**. If **ts_form='unf'** they are read from an unformatted file otherwise as an ASCII formatted file. Either way they are read as global 3D arrays, temperature then salinity:

real*8 temp3d(l,m,n)
read(16) temp3d

or

real*8 temp3d(l,m,n)
real(16,ts_form) temp3d

Alternatively if the **ANALYTIC_INIT** directive is set a FORTRAN file called **tmpfield.F** is 'included'. This should set the values of **tmp** and **sal** at all local b-points. This is useful for defining idealised problems/test cases.

4. Defining forcing for POLCOMS

In all but the most idealised cases external forcing provides an important control on a coastal-ocean simulation. POLCOMS includes a wide range of provisions for surface (metrological), open-boundary (lateral) and riverine/land forcing.

Surface forcing

Complete POLCOMS simulations require surface fluxes of heat (**hfl_in, hfl_out**), momentum (**fs,gs**) and freshwater (**ep**), and also surface pressure, **pr**. Apart from pressure, which is used directly, these are usually defined via bulk formulae from atmospheric data; the alternative approach, to use fluxes directly from an NWP model (e.g. the Met. Office applications of POLCOMS), is not described here. The model then requires the following variables as local arrays (note units):

at air temperature (degrees C)
we,wn wind speed, eastwards and northwards (m/s)
rh relative humidity (%)
cl cloud cover (%)
pr atmospheric pressure (mb)
pn precipitation (ms^{-1})

The data are read in in **metset.F**, which is currently 'hard-wired' to a number of fixed data types. The data is read in on the native grid and frequency of the atmospheric model data set (e.g. as provided by BADC), a copy is passed to each processor and is then interpolated in spaced onto the model grid (this is efficient for coarse resolution atmospheric data, but could be improved with parallel input for large data sets). Note: no distinction between u-points and b-points is made in the interpolation, both use b-point value with the same index. Input infrequency is set by the **istress, icloud, isalt** variables defined in **parameters.dat**.

The model includes code for reading met. data on the Northwest European shelf from two sources. Work in the GCOMS project will generalise this to any region around the globe.

ECMWF data

This is the default and refers to either reanalysis (ERA40) or operational products. Data is read from 3 files: From unit 17, **we, wn, pr, at, rh;** from unit 21. **cl**; from unit 89, **pn**. Optionally solar radiation (**sr**) is read from unit 87. In each case the data is on a grid of size nx x ny = 41x26 staring at -25E, 40N and read from an ASCII file:

read(17,'(10f8.2)') ((modata1(j,k), j=1,nx), k=1,ny)y.

In a number of cases the daily accumulation files (cloud cover, precipitation and solar-radiation) are provided in a 'north to south' format. The directives **FLIPCLD** and **FLIP_PRCP** accommodate this. This data are converted from day^{-1} to s^{-1}

Met. Office data

There are two sources here, differing in resolution: the mesoscale model (~12km; directive **MESOMET**) and a sub-set of the global model data (1^o; directive **GLOBMET**). In each case data is provided as one file per variable. Logical units are:

at	20
pr	17
rh	19
we	18
wn	24
cl	21
ep	15

Note in this case rh is specific humidity rather than relative humidity; this is accounted for in **heatin.F** by the directive **SHUMID.**

The mesoscale data uses unformatted files and has **nx** x **ny** = 218x136 starting at -13E, 48.39N and a resolution of 0.11. The global data sub-set uses formatted files and has **nx** x **ny** = 42x47 starting at -20.4166E, 39.7233N and a resolution of 0.833 lon and 0.5555 lat.

Open boundary forcing

Open boundary forcing consists of elevations and barotropic currents (tidal and residual or combined), and temperature and salinity. A depth varying component of current can also be included in an advective scalar boundary condition. Apart from the radiation component of the barotropic forcing, these are all 'active' boundary conditions in that they require the specification of external values for the variables. This is appropriate for nesting in tidally active flows, but more work on the passive boundary conditions (e.g. implementing an Orlanski condition) is required.

When a model domain is run three files are produced which list the required location of open boundary conditions. These are

openbclist_z	elevation points on the boundary
openbclist_u	velocity points outside the boundary
openbclist_b	elevation points outside the boundary

Each has the format

nzbc	Number of points, nzbc, nzbc,nbbc
ipt jpt	Global index of each open boundary point

.
.
.

ipt jpt(npts)

This then defines the data (and order of the data) required in the open boundary forcing files. The files can be produced by executing the model, but without running any time steps: <exename> -tdur 0, and then used to generate boundary condition data for the first model run.

Tidal forcing

Barotropic tidal elevation and currents are forced using a flux/radiation scheme (with **READ_TIDECON**). Tidal velocities are used to calculate a volume flux into/out of each boundary elevation point, which is used in the standard model equations in ***barot***. The elevation at these grid points is also relaxed towards the imposed tidal elevation at a rate proportional to the long wave phase speed $\sqrt{gh}$ (a 'Flather radiation condition').

Tidal data is provided to the model either according to the lists described above or across the whole of the four boundaries of a rectangular model domain. Information about the tidal constituents to be used is defined in a tidal definition file (unit 43). This has the format:

ncond number of constituents
nfac flag >0 to use date information
idate <hours day month year> corresponding to the start of the model run or series of runs (**start_time**), usually t=0s.
indx which of a standard list of 15 each of 1..ncond tidal constituents refers to. 1) **Q1**, 2) **O1**, 3) **P1**, 4) **S1**, 5) **K1**, 6) **2N2**, 7) **MU2**, 8) **N2**, 9) **NU2**, 10) **M2**, 11) **L2**, 12) **T2**, 13) **S2**, 14) **K2**, 15 **M4**.
mcon =1 or =0 depending on whether each of the **ncond** constituents is to be used

This information is used to apply nodal factors and date corrects to give the correct tidal phase for the specified date. The assumption being the data is provided in date-independent form (if this is not the case set **nfac**=0). The format for the tidal data depends on the whether the **LONGBCFORM** is used. The file (unit 14) starts with the tidal frequencies:

sigma(1) frequency of 1st constituent in degrees/hour
.
.
.
sigma(ncond) frequency of **ncond**th constituent in degrees/hour

then the default is to read:

```
do i=1,ncond
  read(itide,'(8f10.6)') (z1(j,i),j=1,nzbc)
  read(itide,'(8f10.6)') (z2(j,i),j=1,nzbc)
```

```
  read(itide,'(8f10.6)') (u1(j,i),j=1,nubc)
  read(itide,'(8f10.6)') (u2(j,i),j=1,nubc)
  read(itide,'(8f10.6)') (v1(j,i),j=1,nubc)
  read(itide,'(8f10.6)') (v2(j,i),j=1,nubc)
enddo
```

from unit **itide**=14. **z1** and **z2** are the cosine and sine components of the elevation of each constituent (similarly for velocity, **u** and **v**)

If **LONGBCFORM** is used data is read according to

```
do i=1,ncond
  read(itide,'(8f10.6)') (z1(j,i),j=1,nobdZ)
  read(itide,'(8f10.6)') (z2(j,i),j=1,nobdZ)
  read(itide,'(8f10.6)') (u1(j,i),j=1,nobdUV)
  read(itide,'(8f10.6)') (u2(j,i),j=1,nobdUV)
  read(itide,'(8f10.6)') (v1(j,i),j=1,nobdUV)
  read(itide,'(8f10.6)') (v2(j,i),j=1,nobdUV)
enddo
```

where **nobdZ=2l+2m, nobdUV=(2(l+1)+2(m+1)** and the data is ordered east to west and north to south along the southern, northern, eastern then western boundaries (irrespective of whether points are land or sea).

The boundary tidal currents are then calculated from these constituents at each barotropic time step. If directive **ZBAR** is used the equilibrium tide is also used.

Residual/combined forcing

As well as tidal forcing time series of barotropic elevation and current can be applied around the model boundaries. These either represent the residual, in which case they are additive with the tidal component, or they can be used to provide the full forcing. The Data are read from unit **nrm=**77 at a format (default is *, boundzuv_form='unf' for unformatted) and frequency (in hours) set in **parameters.dat** (less than 1 hour currently causes an error). At each time data is read in using

```
  read(nrm,*) (z1(j),j=1,nzbc)
  read(nrm,*) (u1(j),j=1,nubc)
  read(nrm,*) (v1(j),j=1,nubc)
```

and similarly for the unformatted case. **z1, u1, v1** are boundary currents and elevations. These are ramped linearly in time between concurrent values and applied as boundary conditions as described above. A **LONGBCFORM** is also available in a similar format to the tidal constituents.

If only elevations are available these can be imposed using a relaxation condition (set using (**READ_ZET**; this has not been extensively tested).

Temperature and salinity

Two options are provided for scalar boundary conditions, an up-wind advective scheme and a relaxation scheme. Currently the list data format is only available for the advective scheme – the relaxation scheme is limited to the longer format and hence only rectangular domains. The type of T and S boundary condition data is controlled by the file **boundarycon.h**:

```
c #define TS_boundary_condition bost
c #define TS_boundary_condition boundaryTS
#define TS_boundary_condition  boundaryTS_longform
c#define   TS_boundary_condition bfix
c#define   TS_boundary_condition no_bc
```

The appropriate sub-routine is un-commented.

For advective boundary conditions data is provided one grid cell outside the model domain and the boundary condition currents used to advect it into the domain on inflow. Data frequency is set in **parameters.dat** and at each time data is read from unit **nrmt=78** by:

```
do j=1,nbbc
  read(nrmt,*) Iin,Jin,(btmp1(k,j),k=1,n-2)
enddo
do j=1,nbbc
  read(nrmt,*) Iin,Jin,(bsal1(k,j),k=1,n-2)
enddo
```

unless **bounts_form='unf'** in which case

```
do j=1,nbbc
  read(nrmt) (btmp1(k,j),k=1,n-2)
enddo
do j=1,nbbc
  read(nrmt) (bsal1(k,j),k=1,n-2)
enddo
```

is used. Data is ramped linearly in time at each time step.

For relaxation conditions the width of the relaxation zone (**niw**) is set in **parameters.dat**. The relaxation coefficient is set to vary linearly from 1 (clapped) at the open boundary to zero at **niw+1** points in side the model. Data is read uses

```
read(nrmt,*) ((btmp1(k,j),k=1,n-2),j=1,nobw)
read(nrmt,*) ((bsal1(k,j),k=1,n-2),j=1,nobw)
```

where **nobw=2l+2m** unless **VARY_RELAX** is set. In this case the imposed data can vary across the relaxation zone and **nobw=2.niw.l+2.niw.m.** Data is ordered east to west and north to south along the southern, northern, eastern then western boundaries (irrespective of whether points are land or sea). If **VARY_RELAX** is set this is repeated for **kk =1** to **niw** points inside the model domain using the provided data, otherwise the data at the boundary is used across the relaxation zone (note: side length does not decrease as **kk** increases).

A number of FORTRAN program are available to extract boundary condition data from POLCOMS output for use as forcing for a smaller (and usually finer resolution) domain.

River inputs

A simple approach for applying river forcing is used: this is to increase the sea surface elevation according to the volume flux, with a corresponding adjustment to the salinity through the water column. The river locations are provided by an index file (unit 29) that lists the model grid points. The file starts with **nofriv** (number of rivers in the domain) then the locations are given in a range of formats:

Default (36 NW shelf rivers):

read(29,'(i2,1x,a14,2(1x,i3))') idriv(nr),name,icriv(nr),jcriv(nr)

If **NORIVTMP** is set (40 years NW shelf database of ~300 rivers):

read(29,'(i3,2(i4),1x,a20)') idriv(nr),icriv(nr), jcriv(nr),name

If **CEH** set (40 year data base of UK rivers)

read(29,'(i3,1x,a19,2(1x,i3))') idriv(nr),name,icriv(nr),jcriv(nr)

The format for the river data is one row per day and one column per river. The number of rivers in the database (i.e. number of columns) is set in **parameters.dat,** and which of these is in the domain is given by the array **idriv.**

5. Compilation

Compilation is carried out using an application specific script (**make_polcoms**) from the application directory (e.g. **pol3db/setups/plume**). For example:

#!/bin/csh -f

set OPTS = ("-DFLAT -DNOTIDE -DRIVERS -DNO_SCOORD -DADV_BC")
set OPTS = ($OPTS " -DNOCOMPRESS -DANALYTICINIT -DANALYTIC_DEPTH -DANALYTIC_INIT -DRIVERFIX")

set MACHINE = shelf-ibmcluster

```
set POLDIR    =     ../../v6.3
set MAKEDIR = $cwd
set EXE_NAME = shelf

#copy application specific files
cp boundarycon.h       $POLDIR
cp data_out.F          $POLDIR
cp tmpfield.F          $POLDIR
cp set_bathymetry.F    $POLDIR
cp set_mask.F          $POLDIR

#enter source directory
cd  $POLDIR

#compile
#make clean
make $MACHINE  "OPTIONS= $OPTS " “MAKE_TARGET=polcoms”
cd $MAKEDIR

#return to application directory and copy in executable.
cp $POLDIR/$EXE_NAME ./
exit(0)
```

In this example the **OPTS** variable sets a list of complier directives (see appendix A) to define the model problem, use **MACHINE** to choose one of the computer dependent ‘make targets’ in **machine_list,** and the **MAKE_TARGET** variable choose which selection of models is to be compiled. The **makefile** currently includes the following options:

- polcoms
- polcoms_gotm
- polcoms_gotm_ersem
- polcoms_ersem
- polcoms_wam

Each also requires the corresponding cpp directives to be set: **-DERSEM, -DGOTM, -DWAM.**

The optional **make clean** statement will remove all object files and .f files so compilation will start from scratch (usually not necessary).

Compilation proceeds in two stages:

Each FORTRAN source file (**.F**) is compiled in turn by **make:** first compiler directives are resolved to give a **.f** file then these are compiled with the FORTRAN compiler e.g.

cpp –D….. b3drun.F b3drun.f *The resulting .f files should not be edited*

f90 –r8 -c b3drun.F -o b3drun.o

Then all object files (.o) files are linked to create the executable. The default executable name is **shelf**.).

Compilation Options

The make targets in **machine_list** provide the compilation options required for each different computer/compiler. They are also used for different compilation and linking options e.g. for debugging and profiling and to set paths to libraries. Three examples are shown.

A linux workstation with debugging on:

```
shelf-linux-pg-g:
        $(MAKE) $(MAKE_TARGET) "OPTIONS=$(OPTIONS)" \
                "OPTIONS=$(OPTIONS)" "DEBUG=$(DEBUG)" \
                "PROGRAM=$(PROGRAM)" \
                "SIZE=$(SIZE)" "ENV=SERIAL" \
                "CPP=cpp" \
                "CPPFLAGS=-P  -traditional" "CPPMACH=-DLINUX" \
                "CC=pgf90" "CFLAGS=-Ktrap=fp -g" \
                "FC=pgf90" "FFLAGS= -g -r8 -Ktrap=fp -Mprof -Mextend " \
                "OFLAGS=" "GFLAGS=" "PFLAGS=" \
                "LOPTS=  -L /packages/netcdf/netcdf-3.5.1/lib -lnetcdf" \
                "LIBS=$(LIBS)"
```

The POL IBM cluster, using MPI:

```
shelf-ibmcluster-mpi:
        $(MAKE) $(MAKE_TARGET) "OPTIONS=$(OPTIONS)" \
                "OPTIONS=$(OPTIONS)" "DEBUG=$(DEBUG)" \
                "EXE=$(EXE)" \
                "SIZE=$(SIZE)" "ENV=MPI" \
                "CPP=/lib/cpp" \
                "CPPFLAGS=-P -traditional" "CPPMACH=-DLINUX \
-                           -I/usr/local/mpichgm/include/" \
                "CC=mpicc" "CFLAGS= -Ktrap=fp -D_FILE_OFFSET_BITS=64 " \
                "FC=mpif90" "FFLAGS= -r8 -O2 -Mlfs -Ktrap=fp –Mprof
-                           -byteswapio " \
                "OFLAGS=" "GFLAGS=" "PFLAGS=" \
                "LOPTS= -Mprof" \
```

```
                "LIBS=$(LIBS)"
```

The HPCx, IBM Power 5:

```
shelf-regatta-mpi:
        $(PMAKE) $(MAKE_TARGET) \
                "OBJECTS=$(OBJECTS)" "DEPENDS=$(DEPENDS)" \
                "NPES=$(NPES)" \
                "OPTIONS=$(OPTIONS)" "DEBUG=$(DEBUG)" \
                "PROGRAM=$(PROGRAM)" \
                "ENV=MPI" \
                "CPP=/lib/cpp" "CPPFLAGS=-P" "CPPMACH=
I/usr/lpp/ppe.poe/include/thread64 -DIBM" \
                "CC=cc" "CFLAGS=-q64" \
                "FC=mpxlf90_r" "OFLAGS=-O2 -qarch=pwr4 -qtune=pwr4 -qhot -
qsuppress=1500-036" \
                "GFLAGS=" "PFLAGS=" "FFLAGS=-q64" \
                "F77FLAGS=-qfixed" "F90FLAGS=-qsuffix=f=f90" \
                "LFLAGS=-L/usr/local/lib" \
                "LIBS=$(LIBS)"
```

For each new computer POLCOMS is compiled/run on a new target is required in **machine_list**, following this template.

Compiling Additional Models

POLCOMS has been coupled to a range of different modelling systems; notably, ERSEM (ecosystem model), GOTM (turbulence model), CICE (sea ice model) and WAM (wave model). Generally the additional model code is placed in a subdirectory of the POLCOMS source code directory. An objects list file is provided in the POLCOMS directory and 'included' by the makefile. The POLCOMS **makefile** is then used for the additional model (including the **machine_list** options) and all object files created are linked to produce the executable. If there are connections between modules then these need to specified in the **makefile** with a –I option. Note: the dependencies of additional models are not explicitly specified. This means, for example, if a POLCOMS module that the ERSEM model uses is changed, "make clean" should be used for both POLCOMS and ERSEM codes, and the compilation started from scratch. An exception to this procedure is GOTM, which is installed as a library and then linked in.

6. Execution

The mode of execution depends on particular computer used, its job submission system and whether the code is run in batch or interactive mode. Apart from the simplest single processor execution on a stand alone workstation, a batch processing script is required to request resources and control the multi-processor execution.

Runtime arguments

The follow command line options are available (except when the **NOGUI** directive is used):

Model command line options:

-help	: Print this usage information
-quiet	: Suppress stdout monitor
-verbose	: Adds debugging info to monitor
-tdur	: Run length (hours)
-nstep	: Run length (timesteps)
-mnth	: Month number for input
-particles	: Enable particle tracking
-indir	: Directory for input data files
-flipcld	: flips cloud data from north-south to south-north

Restart/checkpointing:

-warm_start	: Start from restart file
-restart	: Start from restart file
-reset	: Resets time, u, v, zet
-restm	: Resets time on restart to start_time
-tchk	: Checkpoint interval (hours)
-nchk	: Checkpoint interval (timesteps)
-tcmin	: Time of first checkpoint (hours)
-ncmin	: Timestep of first checkpoint (hours)
-tfwnd	:Forward-wind input data (hours)

Parallel processing:

-nproc	: Number of processes (not usually required)
-nprocs	: Number of processes ````
-nprocx	: Number of processes in x
-nprocy	: Number of processes in y
-nens	: Number of ensemble members
-asynch	: Use asynchronous comms
-immed	: Use non-blocking comms
-promis	: Use promiscuous receives
-nocomms	: Disable boundary exchange
-noimmed	: Use blocking comms
-nosndrcv	: Do not use send/receive mode
-simple	: Use simple partitioning
-sndrcv	: Use send/receive mode
-synch	: Use synchronous comms
-partrk	: Use RK partitioning
-map	: Print partitioning map to file

Client/Server operation:

-server	: Start POLCOMS as server

Debugging:
-idbg : Debugging point x-coordinate
-jdbg : Debugging point y-coordinate
-kdbg : Debugging point z-coordinate

An important feature available from these run-time options is check-pointing/restarting. For example:
cp filenames.jan01 filenames.dat
./shelf –tdur 744. –tchk 744.
cp filenames.feb01 filenames.dat
./shelf –tdur 672. –tchk 672. -restart
will run **shelf** for two legs (January 2001 and February 2001), check pointing at the end of the first then restarting at the start of the second. This allows a long simulation to be broken down into manageable sections e.g. to fit in the constraints of a batch queuing system.

Parallel Execution

In a normal parallel execution environment in which the number of processors is specified as part of the batch job script or interactive options, POLCOMS picks up the number of processors automatically from the size of the MPI_Comm_World communicator. If necessary the number of processors can be set using the –nprocs command line option. By default, POLCOMS automatically partitions the grid in the two horizontal dimensions using a recursive partitioning algorithm. This balances the number of sea points across the processors in order to obtain the optimum run-time load balance. Usually the default settings are those which will work best and give the best performance. The number of processors is factored in two dimensions as near square as possible e.g. on 8 processors then nprocx=4 and nprocy=2. If a different factorization is required this can be specified using the –nprocx and –nprocy options. The –simple option disables the recursive partitioning in favour of a scheme which divides the domain without any regard to the distribution of sea points. The –map option may be used to write a map of the portioned domain to a file in PPM format. The netpbm package (http://netpbm.sourceforge.net/) may be used to convert this file to an image e.g. using the ppmtogif command. Options –asynch and –synch switch between asynchronous and synchronous communications i.e. normal MPI sends and synchronous MPI sends. Options –immed and –noimmed switch between normal MPI sends and immediate MPI sends. The option –nocomms may be used to disable all nearest neighbour boundary exchange. Whereas this invalidates the results of the code it is useful to compare timings with and without communications.

Running in ensemble mode

It is possible to run POLCOMS in ensemble mode where a number of independent model runs are combined in a single job. To enable this specify the command line option –nens e.g –nens 16. For example when running on 64 processors this will execute 16

independent model runs with 4 processors each (except see later). In order to specify different parameters for each ensemble member POLCOMS looks for individual copies of the files **parameters.dat** and **filenames.dat** of the form **parameters_001.dat**, **parameters_002.dat** etc. and **filenames_001.dat** and **filenames_002.dat** etc. If these files are not found then each ensemble member runs with the same standard **parameters.dat** and **filenames.dat** files. In this way every aspect of the forcing, initial data and output files for the ensemble members may be customized. If different bathymetry files are specified for each ensemble member then POLCOMS reads these first before assigning processors and the number of processors per ensemble member is balanced according to the number of sea points. The standard output from each ensemble member is reassigned to a file named **output_001**, **output_002** etc.

7. Output

POLCOMS has a range of output options controlled by the subroutine ***data_out***. This is an application specific code that is copied into the source directory at compile time, it calls generic output routines contained in **out.F** and **tidemeanout.F.** The general procedure for spatial arrays is to copy data to the **leader** processor (using standard communications routines) and output from here. For output at a specific grid cell, a test is required that that cell is on a particular processor: **if (ielb.le.icg .and. icg.le.ieub .and. jelb.le.jcg .and. jcg.le.jeub) then.** ... The logical units set by **filenames.dat** need to be consistent with those used in data_out.F. Typically a model run uses unformatted compressed binary output for high-volume data (e.g. 3D fields) and formatted output for others. Two examples are described here;

dailymeanUVT

These files are used to output 25 hour means of **tmp**, **sal, u**, and **v**, and also **spm** if used. It can use a compressed format to only output at sea points. In which case, a header is written first containing the size of the grid and the location of the sea b-points. This is repeated for u-points. Then the 3D model fields are output daily. FORTRAN code to read these files is like:

```
real*4, allocatable, dimension (:,:,:) :: tmp,sal,u,v
integer, allocatable, dimension (:) :: isea,jsea,iusea,jusea
.
.
read(1) l,m,n,npsea
if ( .not. allocated(isea)) allocate(isea(npsea),jsea(npsea))
read(1) isea
read(1) jsea

read(1) l,m,n,npusea
if ( .not. allocated(iusea)) allocate(iusea(npusea),jusea(npusea))
read(1) iusea
read(1) jusea
```

```
if ( .not. allocated(tmp) ) then
 allocate(tmp(l,m,n-2))
 allocate(sal(l,m,n-2))
 allocate(u(l,m,n-2))
 allocate(v(l,m,n-2))
endif
do it=1,ntimes
 read(1) itimt
 read(1) ((u(iusea(i),jusea(i),k),k=1,n-2),i=1,npusea)
 read(1) ((v(iusea(i),jusea(i),k),k=1,n-2),i=1,npusea)
 read(1) ((tmp(isea(i),jsea(i),k),k=1,n-2),i=1,npsea)
 read(1) ((sal(isea(i),jsea(i),k),k=1,n-2),i=1,npsea)
```

Note: the binary format of the input and output system must match. As most systems now use IEEE floating point format this is not usually a problem, though there can be an issue with file record structures and big-endian versus little-endian. POLCOMS is generally set up to use UNIX (rather than PC/LINUX) style binaries.

Physseries

This outputs data at a list of grid points typically every hour. The files are opened with,e.g. **call initseries(200,'physseries')**. This will read from unit 88 a list of ioutpt points and for each of this open a file physseries.<i>.RUNID to unit 200+**i**. each call to ***outseries*** (e.g. call outseries_wcol(200,ioutpt)) writes depth profiles of **u,v, tmp, aa, ak, qsq, al** and **spm** if used. Variables are converted to integer unless **REALSERIES** is defined. MATLAB code to read these files is like

```
load physseries…
ni=8
np=length(physseries)/ni;
i=1:np;
t=i/24;
k=2:n-1

ii=ni-1
eval(['clear aa' RunID '_' Id ])
eval(['clear ak' RunID '_' Id ])
eval(['clear qsq' RunID '_' Id ])
eval(['clear al' RunID '_' Id ])

eval(['time' RunID '_' Id '=physseries(ni*i-ii,1);']);
eval(['u' RunID '_' Id '=physseries(ni*i-ii,k)/1000;ii=ii-1;']);
eval(['v' RunID '_' Id '=physseries(ni*i-ii,k)/1000;ii=ii-1']);
eval(['tmp' RunID '_' Id '=physseries(ni*i-ii,k)/1000;ii=ii-1']);
eval(['sal' RunID '_' Id '=physseries(ni*i-ii,k)/1000;ii=ii-1']);
eval(['aa' RunID '_' Id '(:,2:n-1)=physseries(ni*i-ii,k)/100000;ii=ii-1']);
eval(['ak' RunID '_' Id '(:,2:n-1)=physseries(ni*i-ii,k)/100000;ii=ii-1']);
eval(['qsq' RunID '_' Id '(:,2:n-1)=physseries(ni*i-ii,k)/100000;;ii=ii-1']);
```

eval(['al' RunID '_' Id '(:,2:n-1)=physseries(ni*i-ii,k)/1000;;ii=ii-1']);

Work is in progress to replace these files with NetCDF (http://www.unidata.ucar.edu/software/netcdf/).

Appendix A: Model control (CPP directives and logical variables)

Unless otherwise specified the default value of logical variables is .false.

Compiler directive	Logical variable	Description
METOFFICE		Needed if using met. office heat fluxes and system
GULF		A Met. Office domain
AMM		A Met. Office domain
IRSH		A Met. Office domain
MRCS		A Met. Office domain
	advection	Do momentum and scalar advection
	advect_v	Advect v component of momentum
ADV_BC	**adv_bc**	Used advective boundary conditions (otherwise relaxation)
ANALYTIC_DEPTH	**analytic_depth**	Set bathymetry to idealised values defined in set_bathymetry.F
ANALYTIC_INIT	**analytic_init**	Set an analytic buoyancy (temperature) field, defined in tmpfield.F
ATTEN		Use IOP derived attenuation coefficients for heating and ecosystem model
BALTIC	**Baltic**	Include the Baltic as an inflow
BIHARM		Biharmonic, rather than Laplacian in sigma-coordinate horizontal diffusivity (NOT TESTED)

BIO_LAMDA	**bio_lambda**	Use transmissivity from the ERSEM model in the heatflux calculation
BNDUADV		Include boundary points in velocity advection – acts as 'Sommerfeld' type passive boundary condition
BULKMET	**bulk_met**	Read met data from files(s) (pressure, winds, temperature, relative humidity and cloud cover)
BULK_COARE		Use COARE 3 bulk heat flux
BULK_NSP		Use Goldsmith and Bunker Heat bulk heat flux
CEH	**ceh**	Use CEH UK river data
CICE	**cice**	Use the Los Alamos CICE sea ice model
CLOUDPOINT	**cloudpoint**	a single value of cloud data is read to represent the cloud over the whole domain at each time; use with BULKMET
COARSEGRID		Setup a coarse resolution grid to run alongside standard model
COASTFRIC		Increase z0 near coast - not stable
COEF_NSP		Interpolate latitude dependent heat flux parameters
COLLECTIVE		Use collective communication routines
COMPOUT		Only output tide means at sea points
	compress	Use compressibility term in equation of state for HPG.
CONST_TS_BC	**const_ts_bc**	Boundary temperature and salinity values are held constant (values read in from file)
CONST_HORIZ_DIF		Constant diffusivity in σ-coordinate horizontal

		diffusivity, otherwise, Smagorinsky
CONVECTU	**convect_u**	Convective adjustment for u, v, temperature and salinity (not advisable)
CTDTRACK		Output *T*, *S* and SPM profiles according to a list of time, long. and lats.
DEBUG plus extra debugging information on: **DEBUG_MODEL** **DEBUG_ADV** **DEBUG_B3DRUN** **DEBUG_BAROC** **DEBUG_BAROT** **DEBUG_CONVECT** **DEBUG_DIFFUSEB** **DEBUG_DIFFUSEU** **DEBUG_HORIZUV** **DEBUG_HORIZTS** **DEBUG_PGRAD** **DEBUG_LAGRANGE** **DEBUG_EXCHANGE** **DEBUG_COMMS** **DEBUG_GLOBCOM** **DEBUG_LAGRANGE** **DEBUG_STRSET**		Output a range of information and specific values of variables at the debuging point. For use in debugging. physics model advection main program control baroclinic integration barotropic integration convective adjustment scalar diffusion velocity diffusion Horizontal diff. u,v. Horizontal diff T & S. Pressure gradient Particle tracking Halo exchange Communications Global communications Partical tracking Met. Data input
DIA_F	**dia_f**	Output flux data for T and S budget
DIA_T	**dia_t**	Output temperature diagnostics at specified points and in 3D
DSSRDATA		Use downward SW radiation forcing rather than astronomical calculation corrected for clouds. Requires albedo
DSTRDATA		Use downward thermal radiation forcing

DOCUMENT		Make the POLCOMS documentation
ERSEM		Use ERSEM
EXTRARIVS	**extrarivs**	Use constant annual mean data for additional rivers
FOAM		Fix for missing FOAM b.c. data
FORCEafterDIFF		Moving surface forcing to occur after vertical diffusion
FLAT	**Flat**	Use Cartesian coordinates - daldi and dbedi in parameters.dat represent dx and dy in metres.
FLIPBATHY	**flipbathy**	Bathymetry file is read in by row from north to south (default is south to north)
FLIPCLD	**flipcld**	Cloud data is read in by row from south to north (default is north to south)
FLIP_PRCP	**flip_prcp**	Precipitation data is read in by row from south to north (default is north to south)
FLIP_RAD	**flip_rad**	SW radiation data is read in by row from south to north (default is north to south)
GLOBMET	**globmet**	Use Met. Office's Global NWP data
GOTM		Use the General Ocean Turbulence Model to calculate vertical diffusivities
HARM_ANA		Do harmonic analysis and output harmonic constants to file
HARMW		Include the vertical velocity in the harmonic analysis calculations (requires HARM_ANA too)
HORIZDIF	**Horizdif**	Add horizontal diffusion to currents - on Z -levels
HORIZTS	**Horizdifts**	Do horizontal diffusion of

		temperature and salinity (requires HORIZDIF too)
HORIZ_DIF_SIG		Add horizontal diffusion to currents - on σ-levels
HORIZ_DIF_SIG_TS		Do horizontal diffusion of temperature and salinity (requires HORIZ_DIF_SIG too)
	hor_press_grad	Switch on/off hpg
IBM		Machine dependent option for IBM systems (e.g. HPCx)
INVERSE_B	**inverse_b**	Apply inverse barometer correction at the boundary - used when boundary data elevations do not include the effects of atmospheric pressure but either BULKMET or POINTMET is used
IRREG_BC	**irreg_bc**	Use irregular shaped relaxation zone T&S b.c.'s
key_EnKF		Use ensemble Kalman Filter assimilation
Key_EnOI		Use ensemble optimal interpolation assimilation
key_ENSEMBLEOUT		
key_clderr		Perturb cloud cover in ensemble Kalman filter
key_ImpSam		
key_turberr		
key_winderr		
key_1DASSIM		
	lchkpnt	Do full checkpoint at time intervals **tchk**
	lfwnd	Forward-wind forcing data by time **tfwnd**
	lnoout	Suppress output
	looping	
LOCOMS		Run Low resolution Coastal-Ocean Model, in addition to POLCOMS
LONGBCFORM	**longbcform**	use long format boundary conditions - south, north, west, east

	lwarm	Read in full restart data
MPI		Use MPI for message passing
MONITOR		Output largest current speed
MESOMET	**mesomet**	Use Met. Office's mesoscale NWP data
MY25CBF	**my25cbf**	Set a spatially varying coefficient of bottom friction (otherwise constant)
NOCOMPRESS		Omit the pressure term from the calculation of 'potential buoyancy'. Required if not using s-coordinates.
OLD_UR_VR		Use original calculation of depth varying component of volume fluxes in scalar advection
NO_CONVADJ		Do not do a convective adjustment (default with **GOTM** on)
	ncep_lcd	Use cloud data from NCEP (to replace ERA40)
NODIFF	**nodiff**	Switch off vertical diffusion
NOHPG		Switch off horizontal pressure gradient calculation
NOCLI		Make b3drun.F the main program, needed for error trapping with Portland Compilers but disables command line arguments
NOMODEL		Omit the physics model calculations
NO_PGRAD		**C**alculate the horizontal pressure gradientalong σ-levels
NOPHYSADV		Turn off all physics advection
NO_RAMP		Do not ramp up the initial wind forcing
NORIVERSKIP	**riverskip**	Read in river data from

		start of file instead of skipping nday-1 records
NORIVTMP		Do not read in river temperatures
NOROT	**norot**	No rotation - Coriolis force is zero
NO_SAL	**no_sal**	Turn off salinity integration
NOSCAADV	**no_tmp**	Turn off scalar advection
NO_SCOORD	**scoord**	Use σ- rather than s-coordinates
NOSPMADV		Turn off advection of SPM
NOSPMRIV		Turn off spm input from rivers
NOSPMSOURCE	**lspmsource**	Turn off coastal sources of SPM
NOSLIP		
NOSTEEP		Turn off steepening during calculation of horizontal advection
NOSTEEPZ		Turn off steepening during calculation of vertical advection
NOTEVENSIG		σ-levels are not evenly spaced (redundant)
NOTIDE	**no_tide**	Run without tide or residual forcing
NO_TMP		Turn off temperature integration
NO_V		Turn off northwards advection
NOVELADV		Turn off velocity advection
ONESPMADV		Only advect the first SPM class
OUTSCOORD	**outscoord**	Output 3d array of s-coordinates; run will stop as soon as file is written
PARALLEL_STATS		Output parallel statistics
	part_tracking	Use particle tracking sub-model
PGRAD	**lpgrad**	**C**alculate the horizontal pressure gradient by interpolating onto

		horizontal plane (default linear interpolation) Default = .true.
PGRAD_SPLINE	**lpgrad_spline**	Calculate the horizontal pressure by spline interpolation onto horizontal plane
PGRAD_TEST	**pgrad_test**	
	physmodel	Execute the physics model
POINTMET	**point_met**	Use single point met data: pressure, winds, temperature, relative humidity and cloud cover
POLARSTEREO		Use polarstereo project for horizontal coordinates
PROGDENS	**progdens**	Set buoyancy = temperature i.e. equivalent to linear equation of state
PVM		Use PVM for message passing (not recently tested)
Q2L	**q2l**	Use lengthscale equation in MY turbulence closure (not tested)
RAMPTIDE		Increase tidal constituents from zero at start of run
READ_INITIAL_TS	**read_initial_ts**	Read initial temperature and salinity fields from file
READOPENBCPOINTS	**readopenbcpoints**	Read additional open boundary locations from file
READ_TIDECON	**read_tidecon**	Read tidal constituents from file.
READ_ZETUB	**read_zetub**	Read from file boundary elevations and currents at frequency set in **parameters.dat**
READ_ZET	**read_zet**	Read boundary elevations from file for ‘elevation only’ boundary condition
REALSERIES		Use floating point format for time seriesoutput
	reset	Time and currents reset to

		zero – allows spin up of *T* and *S*.
	resetweekmeans	Weekly means are initialized at the start of this run
RILIMIT	**rilimit**	Option on limiting the mixing length in turbulence routines
RIMIX	**rimix**	Use the Richardson number dependent boundary layer mixing scheme
RIVERFIX		Elevation is modified by river inflow at a river grid box during baroclinic (rather than barotropic time step
RIVERS	**rivers**	Include freshwater inflow from rivers
	resettm	Reset time to be **start_time,** rather than time from resart file
SALFLUX	**salflux**	Include salinity flux calculations
SALTFLUX	**lsaltflux**	Read in surface precipitation data
SCOORD_EVEN	**scoord_even**	s-levels are equally-spaced in the vertical (same as σ-levels), irrespective of the water depth
SCOORD		Use horizontally varying vertical coordinate (default: .true.)
SCINTERP		Use original calculation of s-coordinates at u-points
SERIAL		Run on single processor machine
	Server	Run POLCOMS as a server.
SHMEM		Use Cray SHMEM library for message passing in addition to MPI/PVM (not recently tested)
SPM	**lspm**	Use the SPM submodel

	spm_advection	Advect SPM
SSRDATA	**ssrdata**	Use net SW radiation forcing rather than astronomical calculation corrected for clouds
	Stdout	Write monitor output to stdout on this processor
TIMING	**Timing**	Output timing information for various stages of the model run
TIMING_ADV **TIMING_BAROC** **TIMING_BAROT**		Include detailed timing for advection routines Include detailed timing for baroclinic integration Include detailed timing for barotropic integration
TSFLUX		Output horizontal *T* and *S* fluxes
TVD		Use TVD wetting and drying (with WETDRY)
TRACER	**Tracer**	Advection and diffusion of a passive tracer
UBC		Use non-zero tangential velocities at coastal boundaries (for use with case II boundaries)
UBC__CALC		Calculate velocities at coastal-points (with **UCOAST**). Not fully tested
UCOAST	**ucoast**	Use case II boundaries - land boundaries lie along u-points (default is case I)
UNFORMMET	**unformmet**	Use unformatted meteorological data files (specific implementation)
VAMPIR		Use vampire profiler
VARY_LAMBDA	**vary_lambda**	Use a water depth dependent transmissivity in the SW downwelling calculation
VARY_REALAX	**vary_realax**	Use a relaxation boundary condition for temperature and salinity with forcing values changing across the relaxation zone

VECTOR		Use code optimized for vector machine (i.e. not cache optimized)
	Verbose	Write time steps to screen
WAVES	**Waves**	Add wave coupling terms
WAM		Use WAM wave model
WETDRY	**Wetdry**	Use wetting/drying code
WINDFLUC	**Windfluc**	Add a fluctuation component (read in from file) to the wind field
ZBAR	**Lzbar**	Include the equilibrium tide in barotropic calculation
ZERO_PG_BC	**zero_pg_bc**	In the pressure gradient calculation use zero pressure gradient near bed boundary condition (default is zero density gradient)
ZVARYBC	**Zvarybc**	use depth-varying currents in *T* and *S* advective boundary condition

Appendix B: Principle Model variables

Variables defined in module **b3d.F**

Three dimensional arrays

- real*8, dimension(n,1-mhalo:iesub+mhalo,1-mhalo:jesub+mhalo)

Variable	Description	Units	File changed in
aa	Vert. viscosity	m^2s^{-1}	**turbulence.F**
ah	Horiz viscosity	m^2s^{-1}	**horizdiffusivity.F, horizdiffuse.F**
ak	Vert. diffusivity	m^2s^{-1}	**turbulence.F**
aka	Viscosity for slow baroclinic step	m^2s^{-1}	**b3drun.F**
ak_temp	Temporary array	m^2s^{-1}	**b3drun.F**
al	Mixing length	m	**turbulence.F**
b	Buoyancy	ms^{-2}	**bcalc.F**
bsal	Boundary sal.	p.s.u.	**boundaryTS.F**
btmp	Boundary tmp	^oC	**boundaryTS.F**
fu	Volume flux (u)	m^2s^{-1}	**barot.F**

fv	Volume flux (v)	m^2s^{-1}	**barot.F**
fus	Volume flux (u) for slow baroclinic step	m^2s^{-1}	**b3drun.F**
fvs	Volume flux (v) for slow baroclinic step	m^2s^{-1}	**b3drun.F**
qsq	T.K.E.	m^2s^{-2}	**turbulence.F**
sal	Salinity	p.s.u.	**advect_sca.F, saltflux.F, diffuse.F**
tmp	Potential temperature	^oC	**advect_sca.F, downwell.F, diffuse.F**
tra	Tracer	m^{-3}	**advdif_spm.F**
u	Eastward velocity	ms^{-1}	**baroc.F, barot.F diffuse.F, advect_vel.F**
v	Northward velocity	ms^{-1}	**baroc.F, barot.F, diffuse.F, advect_vel.F**
uo	u velocity at last time step	ms^{-1}	**turbulence.F**
vo	v velocity at last time step	ms^{-1}	**turbulence.F**
ur	Depth varying velocity (u)	ms^{-1}	**baroc.F**
vr	Depth varying velocity (v)	ms^{-1}	**baroc.F**
w	Vertical velocity	ms^{-1}	
aln	Mixing length profile	-	**Turbulence.F**
ds	Level	-	**sigmaset.F, scoordset.F**
dsu	Level width	-	**sigmaset.F, scoordset.F**
dsup	Level spacing to surface and sea bed	-	**sigmaset.F, scoordset.F**
dsv	Level width at u-points	-	**scoordset.F**
dsuv	Level spacing at u-points	-	**scoordset.F**
sig	s-levels for state variables, b-point	-	**sigmaset.F, scoordset.F**
sigv	s-levels for state variable, u-point	-	**scoordset.F**
sigo	s-level for flux variable, b-point	-	**sigmaset.F, scoordset.F**
sigov	s-level for flux variable, u-point	-	**scoordset.F**
aastor	25 hours means, aa	m^2s^{-1}	**tidemeanout.F**
akstor	25 hours means, ak	m^2s^{-1}	**tidemeanout.F**

salstor	25 hours means, sal	p.s.u.	**tidemeanout.F**
tmpstor	25 hours means, tmp	^{o}C	**tidemeanout.F**
ustor	25 hours means, u	ms^{-1}	**tidemeanout.F**
vstor	25 hours means, v	ms^{-1}	**tidemeanout.F**
al_stor	25 hours means, al	m	**tidemeanout.F**
spmstor1	25 hour mean, spm1	gm^{-3}	**tidemeanout.F**
spmstor2	25 hour mean, spm2	gm^{-3}	**tidemeanout.F**
tuflx	tmp flux u	$^{o}C\ m^{2}s^{-1}$	**tidemeanout.F**
tvflx	tmp flux v	$^{o}C\ m^{2}s^{-1}$	**tidemeanout.F**
suflx	sal flux u	p.s.u. $m^{2}s^{-1}$	**tidemeanout.F**
svflx	sal flux b	p.s.u. $m^{2}s^{-1}$	**tidemeanout.F**
rowbar	Mean density	kgm^{-3}	**bcalc.F**
pressure	Pressure for compressibility calc.	Pa	**bcalc.F , pgrad.F, p**
d_bl	Worker arrays for advection routines	-	**advpb[uv].F**
d_br	..	-	**advpb[uv].F**
d_dba	..	-	**advpb[uv].F**
d_dmb	..	-	**advpb[uv].F**
d_db	..	-	**advpb[uv].F**
d_d2b		-	**advpb[uv].F**
d_fuu	..	-	**advpb[uv].F**
d_fba	..	-	**advpb[uv].F**
sigo2	..	-	**advpb[uv].F**
Aku	diffusivity at u-point	$m^{2}s^{-1}$	**turbulence.F**
epsilon	Dissipation	$m^{2}s^{-3}$	**turbulence.F**

Two-dimensional arrays at 3 time levels

- real*8, dimension**(1-mhalo:iesub+mhalo,1-mhalo:jesub+mhalo,3)**

Variable	Description	Units	File changed in
Zet	Elevation	m	**barot.F**
Ub	Depth mean current u	ms^{-1}	**barot.F**
Vb	Depth mean current v	ms^{-1}	**barot.F**

Two-dimensional arrays

- real*8, dimension**(1-mhalo:iesub+mhalo,1-mhalo:jesub+mhalo)**

Variable	Description	Units	File changed in

Afnlb	Depth mean of non-linear/buoyancy terms u	ms^{-2}	**baroc.F**
Ar	Fraction area of grid cell	-	**b3dgrid.F**
At	Air temperature	^oC	**metset.F**
Bfnlb	Depth mean of non-linear/buoyancy terms u	ms^{-2}	**baroc.F**
cdb	Bottom friction coefficient	-	**cbfset.F**
Cl	Cloud cover	%	**metset.F**
Csq	'old' bottom friction term	ms^{-1}	**barot.F**
Dzdt	elevation changes	ms^{-1}	**out.F**
Ep	Precipitation minus evaporation	ms^{-1}	**Saltflux.F**
Fb	Bottom stress u	m^2s^{-2}	**barot.F**
Fs	Surface stress u	m^2s^{-2}	**metset.F**
Flxu	Volume flux u	m^2s^{-1}	**tidemeanout.F**
Flxv	Volume flux v	m^2s^{-1}	**tidemeanout..F**
Gb	Bottom stress v	m^2s^{-2}	**barot.F**
Gs	Surface Stress v	m^2s^{-2}	**metset.F**
H	Total water depth	m	**barot.F**
h1	Intermediate water depth	m	**Advect_sca.F**
h2	..	m	**Advect_sca.F**
h22	..	m	**Advect_sca.F**
hfl_in	Heat flux in	$^oCms^{-1}$	**heatin.F**
hfl_out	Heat flux out	$^oCms^{-1}$	**heatin.F**
Hs	Undisturbed water depth	m	**hset.F**
Hsu	Undisturbed water depth u-points	m	**b3dgrid.F**
Hu	Water depth u-points	m	**barot.F**
hu1	Intermediate water depth	m	**Advect_vel.F**
hu2	..	m	**Advect_vel.F**
hu22	..	m	**Advect_vel.F**
Pn	Precipitation	ms^{-1}	**metset.F**
Pr	Atmospheric pressure	mb	**metset.F**
Sr	Shortwave Rad.	Wm^{-2}	**metset.F**
Rh	Relative humidity	%	**metset.F**
Relfac	Relaxation zone factor	-	**bost.F**

We	Eastward wind	ms^{-1}	**metset.F**
Wn	Northward wind	ms^{-1}	**metset.F**
Zbar	Equilibrium tide	m	**tidbndrp2.F**
Zetbc	Elevation boundary condition	m	**tidbndrp2.F, boundaryUVZ.F, bcbr.F**
Dzb	Accumulated change in elevation	m	**barot.F**
Dlim	Limit for equation in very shallow water.	-	**barot_tvd.F**

Two-dimensional integer arrays

- integer, dimension(n,1-mhalo:iesub+mhalo,1-mhalo:jesub+mhalo)

Variable	Description	File changed in
Iapbu	Advection mask	**advset.F**
Iapbv	..	**advset.F**
Iapuu	..	**advset.F**
Iapuv	..	**advset.F**
Incb	point is at open boundary	**setopenbc.F**
Incu	u-point is next to open boundary	**setopenbc.F**
Ipexb	Calculation mask- b	**boset.F**
Ipexu	calculation mask- u	**boset.F**
ipexbb	land-sea mask – b	**boset.F**
ipexub	land sea mask – u	**boset.F**
irel	relaxation zone – points from boundary	**relzone.F**
iucoast	coastal u-point	**b3dgrid.F**

Appendix C: Model parameters

This is an example **parameters.dat** file from the MRCS domain:

```
      251            l    )
      206            m    )   Model grid dimensions
       20            n    )
   10.0d0         hsmin       Minimum water depth
 '(53f6.2)'        bathf       Format for bathymetry
  '(50i2)'        maskf       Format for mask data
 '(20f8.4)'      ts_form       Format for initial temperature & salinity
'(41(1x,f3.0))'                format for cloud data
   '50f8.4'   bounts_form      boundary T S format (only use for =unf)
```

```
    '20f8.4'   bounzuv_form    boundary U,V,zeta format (only use f
      10.0d0        daldi      Inverse longitude resolution (degrees)
      15.0d0        dbedi      Inverse latitude resolution (degrees)
-11.9875d0         along1     Western limit of domain  B-point (1,1)
48.00833d0          alat1     Southern limit of domain B-point (1,
       0.0d0           st      Start time
      20.0d0          dlt      Barotropic time step
          15           mt      Time step ratio
           4          mts      Number of fast baroclinic steps
       744.0         tdur      Run Length
      1.0d-5         avmin     Minimum Diffusivity
     1.0d-15        dbdzmin    Minimum buoyancy gradient in TKE equations.
      1.0d-6         q2min     Minimum turbulent energy
     200.0d0           ahm     Coefficent for Killworth Filter
         0.2           ahc     Coefficient for Smag. or constant h.diff
         1.0           prt     Turbulent Prandlt number
    0.005d0           cbf     Constant or min. coeff. of bottom friction
     3.0d-3            z0     Bottom roughness length
  10000.0d0      conv_lim      Maximum depth for convective adjustment
       0.0d0          land      value for dry land in bathymetry data
       6.0d0       rstress     )
      24.0d0        rcloud     )  Frequency of forcing (hours)
      24.0d0         rsalt     )
           6        ntypes      Number of met. data variables
      24.0d0     bounfreq_TS    Frequency of T and S boundary data (hours)
       1.0d0    bounfreq_ZET    Frequency of U,V,ZET boundary data (hours)
         171            ig     )
         184            jg     )  Debugging co-ordinates
           2            kg     )
       8.0d0       tmp_init     Initial temperature
      35.1d0       sal_init     Initial salinity
          38          noriv     Number of rivers in data base
        0.01           ddry     wetting-drying - depth at which points are 'dry'
         0.5           zwet     change in elevation to next grid point forwetting
           1            niw     Numer of points in relaxation zone.
```

Appendix D: Example compiler directive lists

MRCS – full model

SPM, MY25CBF, READOPENBCPOINTS, RIVERFIX, BULKMET, INVERSE_B RIVERS, TIMING, READ_TIDECON, READ_INITIAL_TS, BALTIC, ADV_BC, CLOUDPOINT, NOSTEEP, ONESPMADV, BNDUADV, SCINTERP, REALSERIES, NOCOMPRESS, PGRAD_SPLINE,VARY_LAMBDA, COMPOUT, CTDTRACK

MRCS – tide only

MY25CBF, READOPENBCPOINTS, NO_TMP, NO_SAL, TIMING, READ_TIDECON, NOSTEEP, BNDUADV, SCINTERP, NOCOMPRESS, NOHPG, COMPOUT, HARM_ANA

HRCS – Full Model

COMPOUT, MY25CBF, BULKMET, NOSTEEP, UCOAST, BALTIC, BNDUADV, VARY_LAMBDA, READOPENBCPOINTS, FLIPCLD, HORIZ_DIF_SIG, HORIZ_DIF_SIG_TS, ADV_BC, NOCOMPRESS, RIVERS, READ_ZETUB TIMING, RIVERS, RIVERFIX, READ_INITIAL_TS, NORIVTMP, ZVARYBC, TRACER, TRACERSTART, BNDUADV, DIA_F, SCINTERP

LB – TVD wetting drying

READ_TIDECON, NO_SCOORD, FLIPBATHY, MY25CBF, NOCOMPRESS, UCOAST, WETDRY, TVD, RIVERS, NO_TMP, NO_PGRAD

S12 – full model

MY25CBF, RIVERFIX, BULKMET, INVERSE_B, RIVERS, READ_TIDECON, READ_INITIAL_TS, BALTIC, NOSTEEP, SALTFLUX, SALFLUX, PGRAD_SPLINE, NOTMPRIV, COMPOUT, TIMING, FLIPCLD, FLIP_PRCP, ZBAR, HORIZTS, HORIZDIF, READ_ZETUB, VARY_REALAX, FLIPBATHY, LONGBCFORM, FOAM, BNDUADV

Plume

BNDUADV, RIVERS, ANALYTIC_INIT, ANALYTIC_DEPTH, FLAT, NO_SCOORD, NOCOMPRESS

Appendix E: Logical units for input data

Unit	File description	Subroutine
13	Mean water depth	***hset***
12	ipexu mask	***boset***
55	Extra open boundary points	***openbcpoints.dat***
16	*T* and *S* initial conditions	***bset***
17	Met. variables for ECMWF forcing	***interp_met1***
21	Cloud data	***interp_met1***
89	Precipitation data	***interp_met1***
87	Shortwave radiation	***interp_met1***
20	air temp	***interp_meso***
17	Pressure	***interp_meso***
19	Humidity	***interp_meso***
18	Eastward wind	***interp_meso***
24	Northward wind	***interp_meso***
15	Precipitation	***interp_meso***

43	Tidal constituents and start time	***tideset***
14	Tidal constituent data	***tideset***
77	Elevation and current boundary data	***boundaryUVZ***
78	T and S boundary data	***boundaryTS***
29	Rivedr index	***fwin***
30	River flow data	***fwin***
31	River water temperature	***fwin***
32	Baltic inflow data	***fwin***
117	River SPM load	***fwin***
88	Time series output points	***filope***

Bibliography

Allen, J. I., J. Blackford, J. T. Holt, R. Proctor, M. Ashworth, and J. Siddorn (2001), A highly spatially resolved ecosystem model for the North West European continental shelf, *SARSIA*, *86*, 423-440.

Ashworth, M., J. T. Holt, and R. Proctor (2004), Optimization of the POLCOMS Hydrodynamic Code for Terascale High-Performance Computers, in *Proceedings of the 18th International Parallel & Distributed Processing Symposium, 26th-30th April 2004*, edited, Santa Fe, New Mexico.

Ashworth, M., R. Proctor, J. T. Holt, J. I. Allen, and J. C. Blackford (2001), Coupled Marine Ecosystem Modelling on High Performance Computers, in *Developments in Teracomputing*, edited by W. Z. a. N. Kreitz, pp. 150-163.

Cooper, W., C. Hinton, N. Ashton, A. Saulter, C. Morgan, R. Proctor, C. Bell, J. Holt, E. Young, and Q. Huggett (2006), UK Marine Renewable Energy Atlas, *ICE Journal of Maritime Engineering*, *In Press*.

Holt, J. T., J. I. Allen, R. Procter, and F. Gilbert (2005), Error quantification of a high resolution coupled hydrodynamic-ecosystem coastal-ocean model: part 1 model overview and assessment of the hydrodynamics *Journal of Marine Systems*, *57*, 167-188.

Holt, J. T., and I. D. James (1999), A simulation of the Southern North Sea in comparison with measurements from the North Sea Project. Part 1: Temperature, *Continental Shelf Research*, *19*, 1087-1112.

Holt, J. T., and I. D. James (1999b), A simulation of the Southern North Sea in comparison with measurements from the North Sea Project. Part 2: Suspended Particulate Matter, *Continental Shelf Research*, *19*, 1617-1642.

Holt, J. T., and I. D. James (2001), An s-coordinate density evolving model of the North West European Continental Shelf. Part 1 Model description and density structure, *Journal of Geophysical Research*, *106(C7)*, 14015-14034.

Holt, J. T., and I. D. James (2006), An assessment of the fine scale-eddies in a high resolution model of the shelf seas west of Great Britain, *Ocean Modelling*, *13*, 271-291.

Holt, J. T., I. D. James, and J. E. Jones (2001), An s-coordinate density evolving model of the North West European Continental Shelf. Part 2 Seasonal currents and tides, *Journal of Geophysical Research*, *106(C7)*, 14035-14053.

Holt, J. T., and R. Proctor (2003), The role of advection in determining the temperature structure of the Irish Sea, *Journal of Physical Oceanography*, *33*, 2288-2306.

Holt, J. T., R. Proctor, J. C. Blackford, J. I. Allen, and M. Ashworth (2004), Advective controls on primary production in the stratified western Irish Sea: an eddy-resolving model study, *Journal of Geophysical Research*, *109*, doi: 10.1029/2003JC001951.

Lewis, K., J. I. Allen, A. Richardson, J, and J. T. Holt (2006), Error quantification of a high resolution coupled hydrodynamic-ecosystem coastal-ocean model: part3, Validation with Continuous Plankton Recorder data, *Journal of Marine Systems*, *63*, 209-224.

Proctor, R., J. T. Holt, J. I. Allen, and J. C. Blackford (2003), Nutrient fluxes and budgets for the North West European Shelf from a three-dimensional model, *Science of the Total Environment*, *313-316*, 769-785.

Proctor, R., J. T. Holt, T. R. Anderson, B. A. Kelly-Gerreyn, J. Blackford, and F. Gilbert (2002), Towards 3-D ecosystem modelling of the Irish Sea., paper presented at Estuarine and Coastal Modeling Proceedings of the 7th International Conference. American Society of Civil Engineers, 5-7 November 2001, St. Petersburg Florida.

Siddorn, J. R., J. I. Allen, J. C. Blackford, F. J. Gilbert, J. T. Holt, M. W. Holt, J. P. Osborne, R. Procter, and D. K. Mills (2007), Modelling the hydrodynamics and ecosystem of the North-West European continental shelf for operational oceanography, *Journal of Marine Systems*, *65*, 417-429.

Young, E. F., and J. T. Holt (2007), Prediction and analysis of long-term variability of temperature and salinity in the Irish Sea, *Journal of Geophysical Research*, *112*, doi:10.1029/2005JC003386, 002007.